Mixed-Integer PDE-Constrained Optimization

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Outline

Mixed-Integer PDE-Constrained Optimization (MIPDECO)

PDE-constrained MIP ... $u = u(t, x, y, z) \Rightarrow$ infinite-dimensional!

- t is time index; x, y, z are spatial dimensions

$$\begin{cases} \underset{u,w}{\text{minimize}} & \mathcal{F}(u, w) \\ \text{subject to} & \mathcal{C}(u, w) = 0 \\ & u \in \mathcal{U}, \quad \text{and} \quad w \in \mathbb{Z}^p \quad \text{(integers)}, \end{cases}$$

- $u(t, x, y, z)$: PDE states, controls, & design parameters
- w discrete or integral variables

MIPDECO Warning

$w = w(t, x, y, z) \in \mathbb{Z}$ may be infinite-dimensional integers!

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It's a MIP, Jim,
but not as we know it!

1st Example Mixed-Integer PDE-Constrained Optimization

Find number and location of sources to match observation $\bar{u}$

$$\begin{cases} \underset{u,w}{\text{minimize}} \quad \mathcal{J} = \frac{1}{2}\int_\Omega (u(w) - \bar{u})^2 d\Omega & \text{least-squares fit} \\ \text{subject to } -\Delta u = \sum_{k,l} w_{kl} f_{kl} \quad \text{in} \quad \Omega & \text{Poisson equation} \\ \qquad \sum_{k,l} w_{kl} \leq S \text{ and } w_{kl} \in \{0,1\} & \text{source budget} \end{cases}$$

with Dirichlet boundary conditions $u = 0$ on $\partial\Omega$.

Example with Gaussian source term, $\sigma > 0$,

$$f_{kl}(x,y) := \exp\left(\frac{-\|(x_k, y_l) - (x,y)\|^2}{\sigma^2}\right),$$

Motivated by porous-media flow application to determine number of boreholes, [Ozdogan, 2004, Fipki and Celi, 2008]

1st Example Mixed-Integer PDE-Constrained Optimization

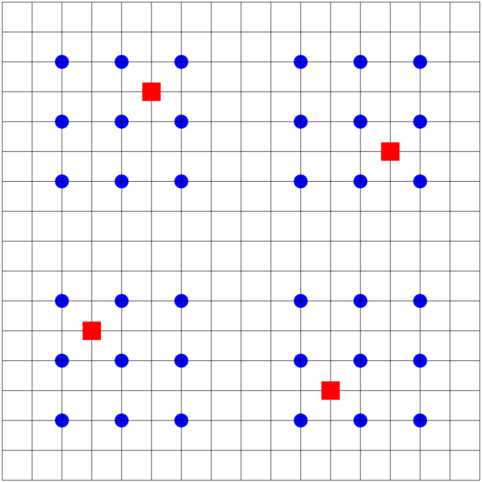
Consider 2D example with $\Omega = [0,1]^2$ and discretize PDE:

- 5-point finite-difference stencil; uniform mesh $h = 1/N$
- Denote $u_{i,j} \approx u(ih, jh)$ approximation at grid points

$$\begin{cases} \underset{u,w}{\text{minimize}} & J_h = \dfrac{h^2}{2} \displaystyle\sum_{i,j=0}^{N} \left(u_{i,j} - \bar{u}_{i,j}\right)^2 \\ \text{subject to} & \dfrac{4u_{i,j} - u_{i,j-1} - u_{i,j+1} - u_{i-1,j} - u_{i+1,j}}{h^2} = \displaystyle\sum_{k,l=1}^{N} w_{kl} f_{kl}(ih, jh) \\ & u_{0,j} = u_{N,j} = u_{i,0} = u_{i,N} = 0 \\ & \displaystyle\sum_{k,l=1}^{N} w_{kl} \leq S \text{ and } w_{kl} \in \{0,1\} \end{cases}$$

$\Rightarrow$ finite-dimensional (convex) MIQP

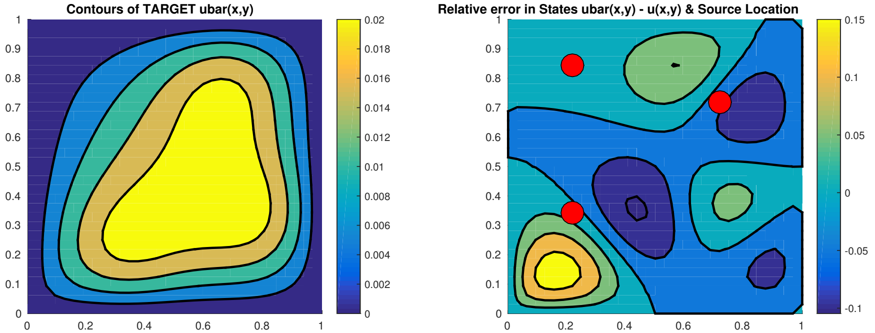
1st Example Mixed-Integer PDE-Constrained Optimization



Potential source locations (blue dots) on 16×16 mesh

Create target $\bar{u}$ using red square sources

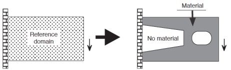
1st Example Mixed-Integer PDE-Constrained Optimization

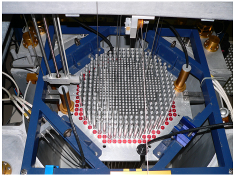


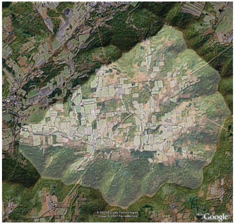
Target (3 sources), reconstructed sources, & error on 32×32 mesh

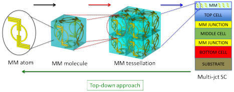
Grand-Challenge Applications of MIPDECO

- Topology optimization [Sigmund and Maute, 2013]
- Nuclear plant design: select core types & control flow rates [Committee, 2010]
- Well-selection for remediation of contaminated sites [Ozdogan, 2004]
- Design of next-generation solar cells [Reinke et al., 2011]
- Design of wind-farms [Zhang et al., 2013]
- Scheduling for disaster recovery: oil-spills [You and Leyffer, 2010] & wildfires [Donovan and Rideout, 2003]
- Design, control & operation of gas networks, see ISMP-TD15, [De Wolf and Smeers, 2000, Martin et al., 2006]
- Design of accelerators ... many more



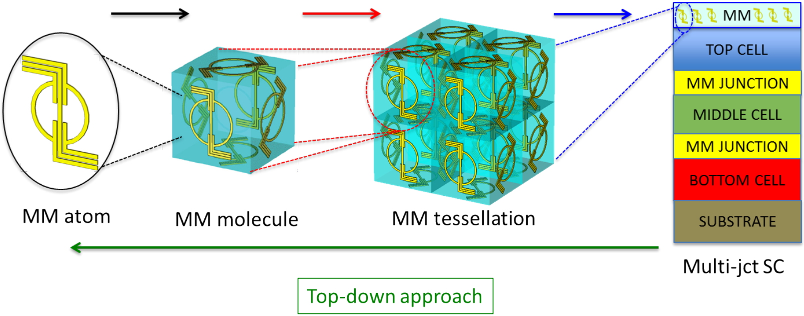






Design of Ultra-Efficient Solar Cell

Design of non-reciprocal optical metamaterial for solar cells



Choose orientation of atoms and molecules to maximize energy

Design of Ultra-Efficient Solar Cell

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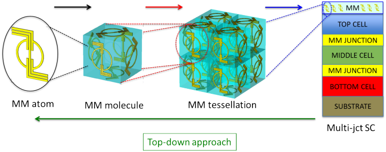


$$\nabla \times \mathbf{H} = -i\omega(\chi \mathbf{H} + \epsilon \mathbf{E}) + \mathbf{J}_e,$$
$$\nabla \times \mathbf{E} = i\omega(\mu \mathbf{H} + \zeta \mathbf{E}) + \mathbf{J}_m,$$

- Maxwell's equation gives **E** and **H** electric and magnetic field
- Objective is to maximize power inside solar cell (x space dims)

$$\frac{1}{2}\int_{\omega} I_{\text{solar}}(\omega) \int_{V} \Im(\epsilon(x,w))|\mathbf{E}(x,w;\omega)|^2 + \Im(\mu(x,w))|\mathbf{H}(x,w;\omega)|^2 \, dV \, d\omega$$

- $w_{i,j,k} = 1$ if orientation i chosen on face j of molecule k
- $w_{i,j,k}$ impact permittivities and permeabilities in Maxwell's

$$\widetilde{\epsilon_{j,k}} = \sum_{i \in \mathcal{O}} w_{i,j,k} \epsilon_i$$

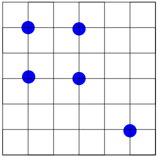
Outline

Mesh-Independent & Mesh-Dependent Integers

Definition (Mesh-Independent & Mesh-Dependent Integers)

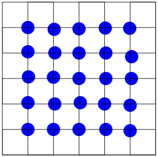
1. The integer variables are mesh-independent, iff number of integer variables is independent of the mesh.
2. The integer variables are mesh-dependent, iff the number of integer variables depends on the mesh.

Mesh-Independent



- Manageable tree size
- Theory possible

Mesh-Dependent



- Exploding tree size
- Theory???

Theoretical Challenges of MIPDECO

Functional Analysis (mesh-dependent integers)

Denis Ridzal: What function space is $w(x, y) \in \{0, 1\}$?

- Consistently approximate $w(x, y) \in \{0, 1\}$ as $h \to 0$?
- Conjecture: $\{w(x, y) \in \{0, 1\}\} \neq L_2(\Omega)$
  ... e.g. binary support of Cantor set not integrable
- Likely need additional regularity assumptions

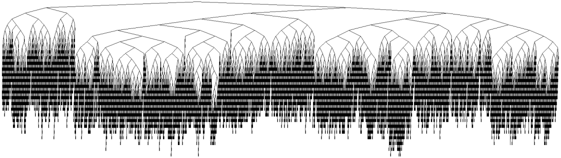
Coupling between Discretization & Integers

Discretization scheme (e.g. upwinding for wave equation) depends on direction of flow (integers).

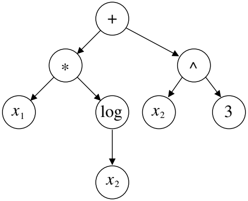
- Application: gas network models with flow reversals

Computational Challenges of MIPDECO

- Approaches for huge branch-and-bound trees
  ... e.g. 3D topology optimization with 10^9 binary variables



- Warm-starts for PDE-constrained optimization (nodes)
- Guarantees for nonconvex (nonlinear) PDE constraints
  ... factorable programming approach hopeless

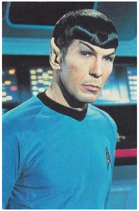


... $f(x_1, x_2) = x_1 \log(x_2) + x_2^3$

MIPDECO: Two Cultures Collide

Observation

PDE-optimization & MIP developed separately
$\Rightarrow$ different assumptions, methodologies, and computational kernels!



PDE-Optimization	**Mixed-Integer Programming**
Obtain good solutions efficiently	Deliver certificate of optimality
Nonlinear optimization: Newton's method	Combinatorial optimization: branch-and-cut
Iterative Krylov solvers	Factors & rank-one updates
Run on bleeding-edge HPC	Limited HPC developments

Potential for Disaster, or Opportunity for Innovation!

Outline

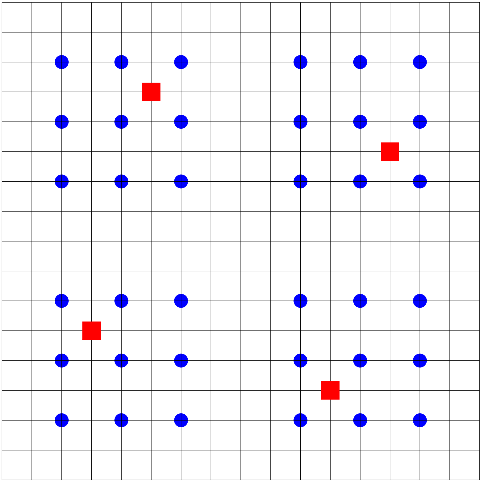
Problem 1: Source Inversion

Find number and location of sources to match observation $\bar{u}$

$$
\begin{cases}
\underset{u,w}{\text{minimize}} \;\; \mathcal{J} = \dfrac{1}{2}\displaystyle\int_\Omega (u(w) - \bar{u})^2 d\Omega & \text{least-squares fit} \\
\text{subject to } -\Delta u = \displaystyle\sum_{k,l} w_{kl} f_{kl} \;\; \text{in} \;\; \Omega & \text{Poisson equation} \\
\qquad \displaystyle\sum_{k,l} w_{kl} \le S \text{ and } w_{kl} \in \{0,1\} & \text{source budget}
\end{cases}
$$

- MIP with convex quadratic objective
- Test NLP-plus-rounding heuristic versus MINLP
- Effect of mesh-dependent vs. mesh-independent integers
  - Mesh-independent: pick sources from 36 potential locations
  - Mesh-dependent: all nodes are potential locations

1st Example Mixed-Integer PDE-Constrained Optimization

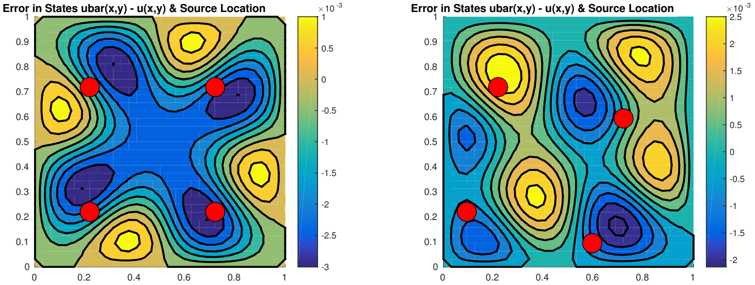


Potential source locations (blue dots) on 16×16 mesh
Create target $\bar{u}$ using red square sources

Approach 1: NLP-Solve, Knapsack Rounding, and MIP

Knapsack Rounding

1. Solve continuous relaxation using NLP solver
2. Solve MILP to find nearest integer & enforce $\sum w_i \le S$

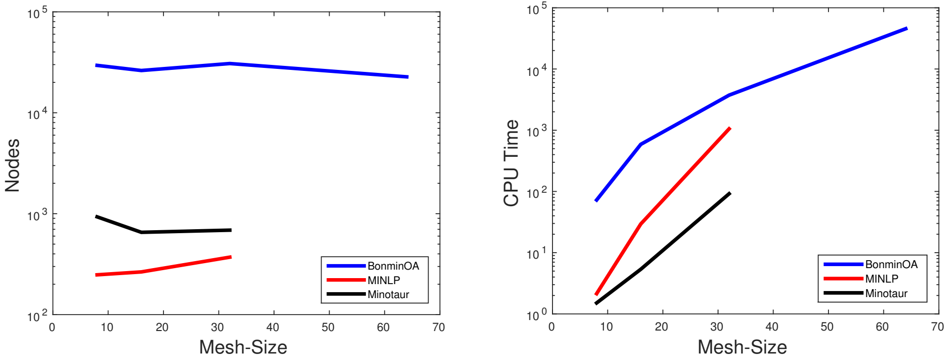


Knapsack-rounded NLP (left) and MINLP (right)

MINLP solution better: NLP-err $= 0.0388 > 0.0307 =$ MIP-err

Mesh-Independent Source Inversion: MINLP Solvers

Number of Nodes and CPU time for Increasing Mesh Sizes



Number of Nodes independent of mesh size!

Mesh-Dependent Source Inversion: MINLP Solvers

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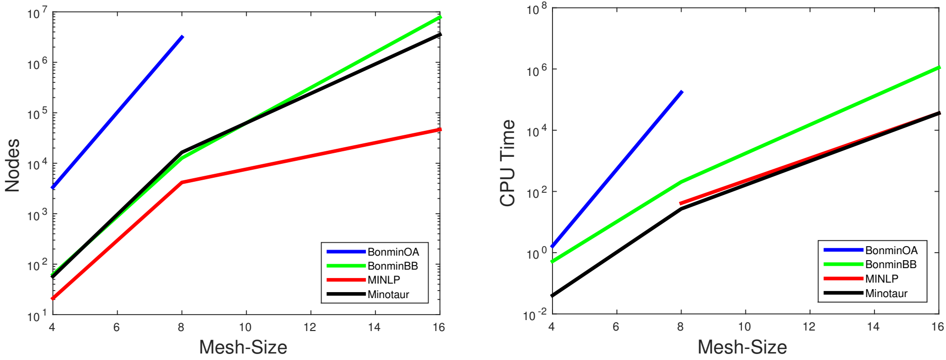


Number of nodes explodes with mesh size!

MIPDECO Trick # 1: Eliminating the PDE

Discretized PDE constraint (Poisson equation)

$$\frac{4u_{i,j} - u_{i,j-1} - u_{i,j+1} - u_{i-1,j} - u_{i+1,j}}{h^2} = \sum_{k,l} w_{kl} f_{kl}(ih, jh), \ \forall i,j$$

$\Leftrightarrow A\mathbf{u} = \sum w_{kl}\mathbf{f}_{kl}$, where $w_{kl} \in \{0,1\}$ only appear on RHS!

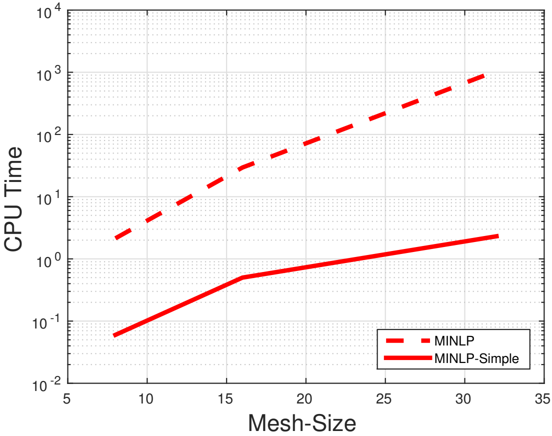
Elimination of PDE and states $u(x,y,z)$

- $A\mathbf{u} = \sum_{k,l} w_{kl}\mathbf{f}_{kl} \ \Leftrightarrow \ \mathbf{u} = A^{-1}\left(\sum_{k,l} w_{kl}\mathbf{f}_{kl}\right) = \sum_{k,l} w_{kl}A^{-1}\mathbf{f}_{kl}$
- Solve $n^2 \ll 2^n$ PDEs: $\mathbf{u}^{(kl)} := A^{-1}\mathbf{f}_{kl}$
- Substitute $\mathbf{u} = \sum_{k,l} w_{kl}\mathbf{u}^{(kl)}$

Simplified model is quadratic knapsack problem

Mesh-Independent Source Inversion (2)

CPU Time for Increasing Mesh Sizes: Simplified vs. Original Model



Eliminating PDEs is two orders of magnitude faster!

Problem 1: Source Inversion

Numerical Results

- Solve mesh-independent problems with coarse discretization
- Mesh-dependent instances cannot be solved
- Outer Approximation (Bon-OA) inefficient for these instances
- Trick # 1: elimination of states and PDE constraint
- Nonlinear solvers run into storage issues

... not surprising: MIPs grow like tribbles!

Problem 1: Source Inversion

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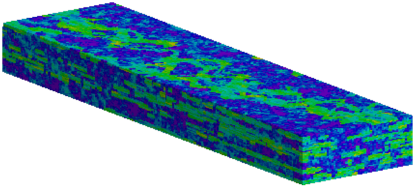
Problem 2: Well Placement & Operation [Bangerth et al., 2006]

Place injection/extraction wells in reservoir to maximize production

- Two-phase flow model with conservation of mass and Darcy's law to model fluxes
- Replace 4^{th} order PDE system by heat equation

$$u_t - K\Delta u = \sum q_s \qquad (1)$$

tensor K models porosity



Porosity Data from spe.org

Maximize net-present value of "production" over $[0, T]$

$$\max_{q,u} \int_{t=0}^{T} (1-d)^{t/T} \sum_{s \in \text{wells}} c_s q_s(t) dt \quad \text{where} d > 0 \text{ discount fact.}$$

Subject to flow model (1) and bounds on wells and flow rates:

$$0 \le q_s(t) \le R w_s, \quad w_s \in \{0,1\}, \quad \sum_s w_s \le U$$

Problem 2: Well Placement & Operation

Discretization of $u(x,t)$ in spatial dimensions x and time t

- 1D instance: Crank-Nicolson (implicit finite-difference)
- 2D instance: 5-point stencil in space, backward Euler in time
- Uniform mesh of size $M \times M$ in space
- Uniform step-size in time with N steps

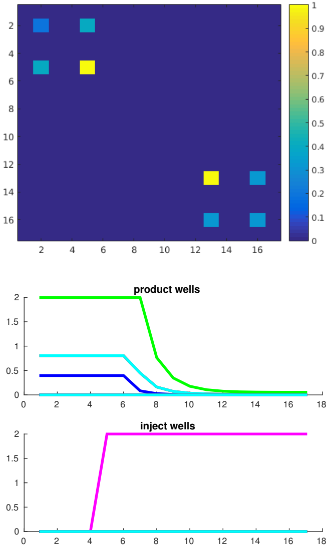
Discretized problem is MILP, i.e. linear

- Number of variables: $\mathcal{O}(M^2 N) = 4096$ for $M = N = 16$, small
- Could again eliminate PDE and states u by
  1. Solving $A\mathbf{u}^{(s)} = \mathbf{e}_s$ for unit vectors $\mathbf{e}_s$ for all wells
  2. Eliminating $\mathbf{u} = \sum q_s \mathbf{u}^{(s)}$ from MILP
- Mesh-independent instances: finite set of possible locations
- Mesh-dependent instances: build wells anywhere

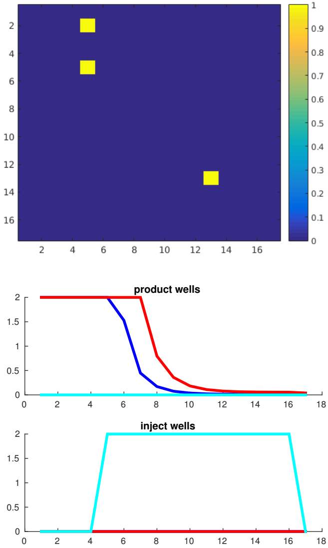
... see also Falk Hante, TD15: Heat Eqn with Actuator Placement

Well Placement & Operation in Two Dimension

Soln of NLP Relaxation



Soln of MINLP



Conclusions

Mixed-Integer PDE-Constrained Optimization (MIPDECO)

- Class of challenging problems with important applications
  - Subsurface flow: oil recovery or environmental remediation
  - Design of next-generation solar cells
- On-going work: Building library of test problems
- Classification: mesh-dependent vs. mesh-independent
- Elimination of PDE and state variables $u(t, x, y, z)$
- Discretized PDEs $\Rightarrow$ huge MINLPs ... push solvers to limit
- Need new ideas, solvers, software for real applications

Outlook and Extensions

- Consider multi-level in space (network) and time
- Move toward truly multi-level approach similar to PDEs

... our five-year mission ...

To boldly go where no optimizer has gone before ...

... to explore strange new PDEs & MIPs!

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